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Variational Method for the Ground State of Multispecies Quantum Fluids*

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A series expansion for the ground-state energy of a multispecies quantum fluid is obtained. This expansion is derived by assuming that the ground-state wave function for the fluid can be approximated by the symmetrized ground-state wave function for a mixture of quantum ideal gases times a product of pair functions. The lowest-order approximation to the energy is minimized with respect to variations in these pair functions in order to obtain an approximation to the ground-state wave function for the system. In principle, this variational procedure can be carried out to any desired order in the energy expansion, and the machinery for doing so is explicitly exhibited. The results of this variation in the lowest order are applied to a two-species system consisting of electrons and nuclei. The results are consistent at high densities.

I. INTRODUCTION

IN recent years, a great deal of attention has been given to the thermodynamic properties of the quantum electron gas. A fair number of techniques have been developed for the treatment of this problem. Some of these are the perturbation expansion which used the Green's-function technique¹⁻³ and another developed by Bohm and Pines⁴ which uses the random-phase approximation (RPA). These techniques give good results at high densities. A variational method has been developed by Gaskell,⁵ who uses collective co-

ordinates and the RPA, which is also good at high densities. Hedin⁶ has combined the RPA and the Martin-Schwinger integral equation to obtain good results in the intermediate density range. The lattice-gas approach^{7,8} holds at low densities.

While attempts have been made to apply the Green's function technique to systems composed of more than one species of particle,⁹ the results are very restricted. A variational method for determining the ground-state properties of multispecies quantum systems is presented in this paper. The method developed here is similar to that used by Gaskell⁵ in his treatment of the quantum electron gas. We assume that the ground-state wave function can be approximated by

$$\psi = \psi_0 \exp\{-\frac{1}{2}\theta\}, \quad (1.1)$$

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¹ M. Gell-Mann and K. A. Brueckner, Phys. Rev. **106**, 364 (1957).

² D. R. DuBois, Ann. Phys. (N. Y.) **7**, 174 (1959).

³ W. J. Carr, Jr. and A. A. Baradudin, Phys. Rev. **133**, A371 (1964).

⁴ D. Bohm and D. Pines, Phys. Rev. **92**, 609 (1953).

⁵ T. Gaskell, Proc. Phys. Soc. (London) **7**, 1182 (1961).

⁶ L. Hedin, Phys. Rev. **139**, A796 (1965).

⁷ E. Wigner, Trans. Faraday Soc. **34**, 678 (1938).

⁸ W. J. Carr, Jr., Phys. Rev. **122**, 1437 (1961).

⁹ H. E. DeWitt, J. Math. Phys. **7**, 616 (1966).

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where θ is a sum of binary functions of the magnitude of the distances between all particles and ψ_0 is some known ground-state wave function for the multispecies system. In principle, ψ_0 can be any function of the coordinates of the particles which is normalized and properly symmetrized so that it will contain the effects which arise from the indistinguishability of identical particles. In practice, we have in mind allowing ψ_0 to be the ground-state wave function for a mixture of n ideal quantum gases, n being the number of species of particles.

When ψ_0 is the ground-state wave function for a mixture of n ideal quantum gases, we can write

$$\psi_0 = \prod_{\alpha=1}^n \psi_0^\alpha, \quad (1.2)$$

where ψ_0^α is the ground-state wave function for an ideal gas composed of the α th species of particle. If the α th species consists of Fermi particles, then ψ_0^α is the Slater determinant of plane waves. If the α th species consists of bosons, then ψ_0^α is unity. Thus any mixture of fermions and bosons can be treated.

Other authors have used trial wave functions of a similar form for one-component systems. Gaskell,⁵ for example, has used exactly this form in his treatment of the electron gas. Others, for example, Woo,¹⁰ who treats He³ atoms, have used a form in which $e^{-\theta/2}$ is a solution to a system of interacting bosons. While this approach is valid for the treatment of interatomic potentials, such as the Lennard-Jones potential, it neglects the effects of symmetry upon $e^{-\theta/2}$ and is inadequate for the treatment of potentials such as the Coloumb potential.

A series expansion for the energy is derived which can be minimized with respect to variations in θ to determine the ground-state wave function for the system. We illustrate the variational procedure by applying it to the lowest-order term in the energy expansion. The machinery for doing so is explicitly exhibited.

The solution in the lowest-order approximation for the one-species system is identical to that of Gaskell.⁵ We also obtain the solution for the two-species system and apply it to a system composed of electrons and nuclei. It is found that it is appropriate to write the energy as the sum of the electron-gas energy plus the nuclei-gas energy plus a term which represents the interaction between the electrons and the nuclei. Since the lowest-order approximation to the energy is equivalent to the RPA plus the Broyles-Sahlin¹¹ (BS) approximation for the pair-correlation functions, these results are expected to be good at high densities. However, at low densities we know that the BS approximation is not valid, and thus these results would not be expected to hold.

We also explicitly evaluate the energy of a two-species

system composed of electrons and spin- $\frac{1}{2}$ nuclei at high densities. It is easy to repeat this calculation for a system composed of electrons and Bose nuclei, for example, He⁴ at high densities.

II. ENERGY OF THE SYSTEM

We shall consider the system to be composed of n species of particles in a box of volume V . There are N_1 particles of mass m_1 , N_2 particles of mass m_2 , up to N_n particles of mass m_n . The Hamiltonian for the system can be written as

$$H = - \sum_{\alpha=1}^n \sum_{j=1}^{N_\alpha} \frac{\hbar^2}{2m_\alpha} \nabla_{\alpha j}^2 + U, \quad (2.1)$$

where \hbar is Planck's constant divided by 2π , $\nabla_{\alpha j}^2$ is the Laplacian with respect to the j th particle of the α th species,¹² and the U is the potential-energy operator. In general, U depends upon the coordinates of all the particles and is here assumed to be an algebraic operator.

The Hamiltonian is now rewritten in the form

$$H = H_0 + U', \quad (2.2)$$

where

$$H_0 = - \sum_{\alpha=1}^n \sum_{j=1}^{N_\alpha} \frac{\hbar^2}{2m_\alpha} \nabla_{\alpha j}^2 + U, \quad (2.3)$$

and

$$U' = U - U_0. \quad (2.4)$$

For the present, U_0 is an arbitrary algebraic potential. In order to proceed with the calculations, we must now solve the equation

$$H_0 \psi_0 = E_0 \psi_0 \quad (2.5)$$

for the eigenvalue E_0 and the eigenfunction ψ_0 , corresponding to the ground state of the system. The eigenfunction ψ_0 is normalized and must be symmetrized so that it is symmetric upon the interchange of identical bosons and antisymmetric upon the interchange of identical fermions. In practice, we are able at the present time to solve Eq. (2.5) only for the case in which U_0 is zero (i.e., the ideal quantum gas). However, for the sake of generality, we shall allow U_0 to remain arbitrary throughout the formalism.

If we choose the eigenfunction ψ_0 to be real, then we can write the real ground-state wave function for the total system as

$$\psi = \psi_0 e^{-\theta/2}, \quad (2.6)$$

where θ is a real symmetric function of the coordinates of all of the particles. In terms of the wave function ψ , the expression for the energy of the ground state of the system is given by

$$E = \frac{1}{Q} \int \psi H \psi d\tau = \langle H \rangle, \quad (2.7)$$

¹⁰ C. W. Woo, Phys. Rev. 151, 138 (1966).

¹¹ A. A. Broyles and H. L. Sahlin, Bull. Am. Phys. Soc. 8, 32 (1963); A. A. Broyles, H. L. Sahlin, and D. D. Carley, Phys. Rev. Letters 10, 319 (1913).

¹² We have adopted the convention of using Greek indices for numbering the species, while using Roman indices for numbering the particles of a given species.

where

$$Q = \int \psi^2 d\tau. \quad (2.8)$$

The notation $d\tau$ stands for the supervolume element given by

$$d\tau = \prod_{\alpha=1}^n \prod_{j=1}^{N_{\alpha}} d\tau_{\alpha j}, \quad (2.9)$$

where $d\tau_{\alpha j}$ is the volume element corresponding to the j th particle of the α th species.

Using Eqs. (2.1), (2.2), and (2.6), we can write

$$\begin{aligned} H\psi = e^{-\theta/2} (H_0\psi_0) - 2 \sum_{\alpha=1}^n \sum_{j=1}^{N_{\alpha}} \frac{\hbar^2}{2m_{\alpha}} (\nabla_{\alpha j} e^{-\theta/2}) \cdot (\nabla_{\alpha j} \psi_0) \\ - \sum_{\alpha=1}^n \sum_{j=1}^{N_{\alpha}} \frac{\hbar^2}{2m_{\alpha}} \psi_0 \nabla_{\alpha j}^2 e^{-\theta/2} + U' \psi_0 e^{-\theta/2}. \end{aligned} \quad (2.10)$$

Then, from Eqs. (2.5) and (2.7),

$$\begin{aligned} E = E_0 - \sum_{\alpha=1}^n \sum_{j=1}^{N_{\alpha}} \frac{\hbar^2}{2m_{\alpha}} Q^{-1} \int [e^{-\theta/2} (\nabla_{\alpha j} \psi_0^2) \cdot (\nabla_{\alpha j} e^{-\theta/2}) \\ + \psi_0^2 e^{-\theta/2} \nabla_{\alpha j}^2 e^{-\theta/2}] d\tau + \langle U' \rangle, \end{aligned} \quad (2.11)$$

where we have used

$$\psi_0 e^{-\theta/2} (\nabla_{\alpha j} \psi_0) = \frac{1}{2} e^{-\theta/2} (\nabla_{\alpha j} \psi_0^2). \quad (2.12)$$

Equation (2.11) can be simplified by writing

$$\begin{aligned} e^{-\theta/2} (\nabla_{\alpha j} \psi_0^2) \cdot (\nabla_{\alpha j} e^{-\theta/2}) + \psi_0^2 e^{-\theta/2} \nabla_{\alpha j}^2 e^{-\theta/2} \\ = \nabla_{\alpha j} \cdot (\psi_0^2 e^{-\theta/2} \nabla_{\alpha j} e^{-\theta/2}) - \psi_0^2 (\nabla_{\alpha j} e^{-\theta/2}) \cdot (\nabla_{\alpha j} e^{-\theta/2}) \\ = -\frac{1}{2} \nabla_{\alpha j} \cdot (\psi_0^2 \nabla_{\alpha j} \theta) - \frac{1}{4} \psi_0^2 (\nabla_{\alpha j} \theta) \cdot (\nabla_{\alpha j} \theta), \end{aligned} \quad (2.13)$$

in which case the energy becomes

$$\begin{aligned} E = E_0 + \left\langle -\frac{1}{4} \sum_{\alpha=1}^n \sum_{j=1}^{N_{\alpha}} \frac{\hbar^2}{2m_{\alpha}} (\nabla_{\alpha j} \theta) \cdot (\nabla_{\alpha j} \theta) + U' \right\rangle \\ + \frac{1}{2} \sum_{\alpha=1}^n \sum_{j=1}^{N_{\alpha}} \frac{\hbar^2}{2m_{\alpha}} Q^{-1} \int \nabla_{\alpha j} \cdot (\psi_0^2 \nabla_{\alpha j} \theta) d\tau. \end{aligned} \quad (2.14)$$

The last term in this equation represents surface effects which can be neglected as the volume becomes large. Thus the expression for the energy is given by

$$E = E_0 + \left\langle -\frac{1}{4} \sum_{\alpha=1}^n \sum_{j=1}^{N_{\alpha}} \frac{\hbar^2}{2m_{\alpha}} (\nabla_{\alpha j} \theta) \cdot (\nabla_{\alpha j} \theta) + U' \right\rangle. \quad (2.15)$$

Equation (2.15) is a complete general expression for the energy. If we now minimize the energy with respect to variations in θ , we could in principle solve for θ , and thus for the ground-state wave function for the system. To attempt this variation without approximation would indeed be an overwhelming task. We therefore choose to approximate θ as a sum of pair functions which depend

only upon the separation of individual pairs of particles. This approximation appears to introduce very little error, and its use has been widespread.

Our calculation will be facilitated by expressing θ as a Fourier series. With this in mind, we begin by noting that with the pair approximation, θ can be written in terms of its Fourier components as

$$\theta = \frac{1}{2V} \sum_{\mathbf{K}} \mathbf{P}^\dagger(\mathbf{K}) \Phi(\mathbf{K}) \mathbf{P}(\mathbf{K}). \quad (2.16)$$

In Eq. (2.16), the $\mathbf{P}(\mathbf{K})$ are n -dimensional *column* vectors given by

$$\mathbf{P}(\mathbf{K}) = [\rho_1(\mathbf{K}) \cdots \rho_{\alpha}(\mathbf{K}) \cdots \rho_n(\mathbf{K})], \quad (2.17)$$

where

$$\rho_{\alpha}(\mathbf{K}) = \sum_{j=1}^{N_{\alpha}} \exp\{i\mathbf{K} \cdot \mathbf{r}_{\alpha j}\} \quad (2.18)$$

are collective coordinates for the α th species and the dagger stands for Hermitian adjoint.¹³ The $\Phi(\mathbf{K})$ are $n \times n$ matrices whose elements are given by the Fourier transform

$$\phi_{\alpha\beta}(\mathbf{K}) = \int \theta(\mathbf{r}) e^{i\mathbf{K} \cdot \mathbf{r}} d\mathbf{r}. \quad (2.19)$$

By using the fact that θ is real and depends only upon the separation of individual pairs of particles, it is easy to show that the $\Phi(\mathbf{K})$ are real symmetric matrices and, in addition, satisfy the relation

$$\Phi(\mathbf{K}) = \Phi(-\mathbf{K}). \quad (2.20)$$

From Eq. (2.16) we can write

$$\begin{aligned} \nabla_{\alpha j} \theta = \frac{1}{2V} \sum_{\mathbf{K}} [\mathbf{P}^\dagger(\mathbf{K}) \Phi(\mathbf{K}) (\nabla_{\alpha j} \mathbf{P}(\mathbf{K})) \\ + (\nabla_{\alpha j} \mathbf{P}^\dagger(\mathbf{K})) \Phi(\mathbf{K}) \mathbf{P}(\mathbf{K})] \end{aligned} \quad (2.21)$$

or

$$\nabla_{\alpha j} \theta = \frac{i}{2V} \sum_{\mathbf{K}} \mathbf{K} [\mathbf{P}^\dagger(\mathbf{K}) \Phi(\mathbf{K}) \mathbf{P}_{\alpha j}(\mathbf{K}) - \mathbf{P}_{\alpha j}^\dagger(\mathbf{K}) \Phi(\mathbf{K}) \mathbf{P}(\mathbf{K})], \quad (2.22)$$

where we have the column vector

$$\mathbf{P}_{\alpha j}(\mathbf{K}) = [0 \cdots \exp(i\mathbf{K} \cdot \mathbf{r}_{\alpha j}) \cdots 0]. \quad (2.23)$$

Now, by using Eq. (2.22), we can write

$$\begin{aligned} \sum_{\alpha=1}^n \sum_{j=1}^{N_{\alpha}} \frac{\hbar^2}{2m_{\alpha}} (\nabla_{\alpha j} \theta) \cdot (\nabla_{\alpha j} \theta) = -\frac{1}{4V^2} \sum_{\mathbf{K}\mathbf{L}} \mathbf{K} \cdot \mathbf{L} \sum_{\alpha=1}^n \sum_{j=1}^{N_{\alpha}} \frac{\hbar^2}{2m_{\alpha}} \\ \times [\mathbf{P}^\dagger(\mathbf{K}) \Phi(\mathbf{K}) \mathbf{P}_{\alpha j}(\mathbf{K}) - \mathbf{P}_{\alpha j}^\dagger(\mathbf{K}) \Phi(\mathbf{K}) \mathbf{P}(\mathbf{K})] \\ \times [\mathbf{P}^\dagger(\mathbf{L}) \Phi(\mathbf{L}) \mathbf{P}_{\alpha j}(\mathbf{L}) - \mathbf{P}_{\alpha j}^\dagger(\mathbf{L}) \Phi(\mathbf{L}) \mathbf{P}(\mathbf{L})]. \end{aligned} \quad (2.24)$$

After some tedious but straightforward manipulation,

¹³ In this paper, we denote matrices by boldface upper-case letters and matrix elements by the corresponding lower-case letter.

Eq. (2.24) reduces to

$$\sum_{\alpha=1}^n \sum_{j=1}^{N_{\alpha}} \frac{\hbar^2}{2m_{\alpha}} (\nabla_{\alpha j} \theta) \cdot (\nabla_{\alpha j} \theta) = \frac{\hbar^2}{2m_1 V} \sum_{\mathbf{K}\mathbf{L}} \mathbf{K} \cdot \mathbf{L} \times [\mathbf{P}^\dagger(\mathbf{K}) \Phi(\mathbf{K}) \Xi(\mathbf{K}-\mathbf{L}) \Phi(\mathbf{L}) \mathbf{P}(\mathbf{L})], \quad (2.25)$$

where $\Xi(\mathbf{K}-\mathbf{L})$ are $n \times n$ matrices whose elements are given by

$$\xi_{\alpha\beta}(\mathbf{K}-\mathbf{L}) = \delta_{\alpha\beta} \frac{m_1 \rho_{\alpha}(\mathbf{K}-\mathbf{L})}{m_{\alpha} V} \quad (2.26)$$

and $\delta_{\alpha\beta}$ is the Kronecker delta. Using Eq. (2.25), the expression for the energy becomes

$$E = E_0 + \left\langle \frac{\hbar^2}{8m_1 V} \sum_{\mathbf{K}\mathbf{L}} \mathbf{K} \cdot \mathbf{L} \times [\mathbf{P}^\dagger(\mathbf{K}) \Phi(\mathbf{K}) \Xi(\mathbf{K}-\mathbf{L}) \Phi(\mathbf{L}) \mathbf{P}(\mathbf{L})] + U' \right\rangle. \quad (2.27)$$

If the potential U' is a sum of pair functions (for example, the Coulomb potential), then it can be written as

$$U' = \frac{\hbar^2}{8m_1 V} \times \sum_{\mathbf{K}} K^2 \{ \mathbf{P}^\dagger(\mathbf{K}) \mathbf{M}(\mathbf{K}) \mathbf{P}(\mathbf{K}) - \sum_{\alpha} N_{\alpha} \mu_{\alpha\alpha}(\mathbf{K}) \}. \quad (2.28)$$

Here the $\mathbf{M}(\mathbf{K})$ are $n \times n$ real symmetric matrices whose elements are given by

$$\mu_{\alpha\beta}(\mathbf{K}) = \frac{4m_1}{\hbar^2 K^2} \int U'(\mathbf{r}) e^{-i\mathbf{K} \cdot \mathbf{r}} d\mathbf{r}. \quad (2.29)$$

As was the case with $\Phi(\mathbf{K})$, it can be shown that

$$\mathbf{M}(\mathbf{K}) = \mathbf{M}(-\mathbf{K}). \quad (2.30)$$

The second term in Eq. (2.28) represents the self-energy of the particles and must be subtracted out in order to use the $\mathbf{P}(\mathbf{K})$. It is, however, simply a constant, which we shall represent by E_* . Using Eq. (2.28), the expression for the energy given by Eq. (2.27) becomes

$$E = E_0 - E_* + \frac{\hbar^2}{8m_1 V} \sum_{\mathbf{K}} K^2 \times \langle \mathbf{P}^\dagger(\mathbf{K}) [\Phi(\mathbf{K}) \Xi(0) \Phi(\mathbf{K}) + \mathbf{M}(\mathbf{K})] \mathbf{P}(\mathbf{K}) \rangle - \frac{\hbar^2}{8m_1 V} \times \sum'_{\mathbf{K}\mathbf{L}} \mathbf{K} \cdot \mathbf{L} \langle \mathbf{P}^\dagger(\mathbf{K}) \Phi(\mathbf{K}) \Xi^*(\mathbf{K}+\mathbf{L}) \Phi(\mathbf{L}) \mathbf{P}(\mathbf{L}) \rangle, \quad (2.31)$$

where the notation $\sum'_{\mathbf{K}\mathbf{L}}$ means that $\mathbf{K} = -\mathbf{L}$ is omitted from the double sum, and the asterisk means complex conjugate.

For reasons which will be clear later, it is desirable to rewrite the last term in this equation so that the sums over \mathbf{K} and \mathbf{L} are restricted to values of \mathbf{K} and \mathbf{L} for which $K_z > L_z > 0$, where K_z is the z component of the vector \mathbf{K} . When this is done, Eq. (2.31) becomes

$$E = E_0 - E_* + \frac{\hbar^2}{8m_1 V} \sum_{\mathbf{K}} K^2 \times \langle \mathbf{P}^\dagger(\mathbf{K}) [\Phi(\mathbf{K}) \Xi(0) \Phi(\mathbf{K}) + \mathbf{M}(\mathbf{K})] \mathbf{P}(\mathbf{K}) \rangle - \frac{\hbar^2}{2m_1 V} \sum_{K_z > L_z > 0} \mathbf{K} \cdot \mathbf{L} \text{Re} \langle \mathbf{P}^\dagger(\mathbf{K}) \Phi(\mathbf{K}) \Xi^*(\mathbf{K}+\mathbf{L}) \Phi(\mathbf{L}) \mathbf{P}(\mathbf{L}) - \mathbf{P}^\dagger(\mathbf{K}) \Phi(\mathbf{K}) \Xi(\mathbf{K}-\mathbf{L}) \Phi(\mathbf{L}) \mathbf{P}(\mathbf{L}) \rangle, \quad (2.32)$$

where Re stands for the real part of the function.

Unfortunately, at this point it is necessary to drop the matrix notation. If we employ the usual convention of summation over repeated Greek indices, then Eq. (2.32) becomes

$$E = E_0 - E_* + \frac{\hbar^2}{8m_1 V} \sum_{\mathbf{K}} K^2 [\phi_{\alpha\beta}(\mathbf{K}) g_{\beta} \phi_{\beta\gamma}(\mathbf{K}) + \mu_{\alpha\gamma}(\mathbf{K})] \times \langle \rho_{\alpha}^*(\mathbf{K}) \rho_{\gamma}(\mathbf{K}) \rangle - \frac{\hbar^2}{2m_1 V^2} \sum_{K_z > L_z > 0} \mathbf{K} \cdot \mathbf{L} \phi_{\alpha\beta}(\mathbf{K}) \frac{m_1}{m_{\beta}} \times \phi_{\beta\gamma}(\mathbf{L}) \text{Re} \langle \rho_{\alpha}(\mathbf{K}) \rho_{\beta}^*(\mathbf{K}+\mathbf{L}) \rho_{\gamma}(\mathbf{L}) - \rho_{\alpha}^*(\mathbf{K}) \rho_{\beta}(\mathbf{K}-\mathbf{L}) \rho_{\gamma}(\mathbf{L}) \rangle, \quad (2.33)$$

where

$$g_{\beta} = (m_1/m_{\beta}) \rho_{\beta}^0 \quad (2.34)$$

and ρ_{β}^0 is the density of particles of the β th species. The integrals

$$\langle \rho_{\alpha}^*(\mathbf{K}) \rho_{\beta}(\mathbf{K}) \rangle = Q^{-1} \int \rho_{\alpha}^*(\mathbf{K}) \rho_{\beta}(\mathbf{K}) \psi^2 d\tau \quad (2.35)$$

and

$$\begin{aligned} & \text{Re} \langle \rho_{\alpha}(\mathbf{K}) \rho_{\beta}^*(\mathbf{K}+\mathbf{L}) \rho_{\gamma}(\mathbf{L}) - \rho_{\alpha}^*(\mathbf{K}) \rho_{\beta}(\mathbf{K}-\mathbf{L}) \rho_{\gamma}(\mathbf{L}) \rangle \\ &= \text{Re} Q^{-1} \int [\rho_{\alpha}(\mathbf{K}) \rho_{\beta}^*(\mathbf{K}+\mathbf{L}) \rho_{\gamma}(\mathbf{L}) - \rho_{\alpha}^*(\mathbf{K}) \rho_{\beta}(\mathbf{K}-\mathbf{L}) \rho_{\gamma}(\mathbf{L})] \psi^2 d\tau \end{aligned} \quad (2.36)$$

depend upon the $\Phi(\mathbf{K})$, and this dependence must be known before our variational procedure can be applied to Eq. (2.33). In Sec. III, a method for evaluating integrals of the type given by Eqs. (2.35) and (2.36) is discussed, and by using this method a series for the energy is obtained in which the dependence of each term upon the $\Phi(\mathbf{K})$ is known.

III. EVALUATION OF INTEGRALS AND ENERGY EXPANSION

The route taken in order to obtain the energy is somewhat circuitous, and the notation has a tendency to be cumbersome. In order to help prevent the reader from being distracted by the mathematics which follows, some preliminary discussion of this section is desirable.

If one views the integrals in Eqs. (2.35) and (2.36) simply as functions of the $\Phi(\mathbf{K})$, which enter through ψ^2 , the energy expression in Eq. (2.33) is in a fairly simple form. The entire complexity of the problem is associated with expressing these integrals as known functions of the $\Phi(\mathbf{K})$. Section III A is devoted to the development of a method by which this can be accomplished. The final expression for these integrals is in the form of a series expansion. In Sec. III B, the results of Sec. III A are used to expand the energy as a series. The formal expression for this energy is fairly complicated. Fortunately, much of the complexity disappears when we examine it term by term.

A. Evaluation of the Integrals

Equations (2.35) and (2.36) are special cases of integrals of the general form

$$I[F(\mathbf{P})] = \int F(\mathbf{P}) \times \exp \left[-\frac{1}{2V} \sum_{\mathbf{K}} \mathbf{P}^\dagger(\mathbf{K}) \Phi(\mathbf{K}) \mathbf{P}(\mathbf{K}) \right] \psi_0^2 d\tau, \quad (3.1)$$

where $F(\mathbf{P})$ stands for a function of any number of the collective coordinates $\rho_\alpha(\mathbf{K})$, and ψ^2 has been replaced by the expressions in Eqs. (1.1) and (2.16). We thus direct our attention to the evaluation of this integral.

It is convenient at this point to transform the complex variables $\mathbf{P}(\mathbf{K})$ to a set of real variables $\mathbf{X}(\mathbf{K})$ defined by¹⁴

$$\mathbf{X}(\mathbf{K}) = (2V)^{-1/2} [\mathbf{P}(\mathbf{K}) + \mathbf{P}^*(\mathbf{K})], \quad K_z > 0$$

and

$$\mathbf{X}(\mathbf{K}) = -i(2V)^{-1/2} [\mathbf{P}(\mathbf{K}) - \mathbf{P}^*(\mathbf{K})], \quad K_z < 0.$$

Using Eqs. (3.2), the integral in Eq. (3.1) becomes

$$I[F(\mathbf{P})] = \int F(\mathbf{P}(\mathbf{X})) \times \exp \left\{ -\frac{1}{2} \sum_{\mathbf{K}} \mathbf{X}^\dagger(\mathbf{K}) \Phi(\mathbf{K}) \mathbf{X}(\mathbf{K}) \right\} \psi_0^2 d\tau. \quad (3.3)$$

Note that the definition of $\mathbf{X}(\mathbf{K})$ changes when K_z changes sign. This is the reason for writing the last term in Eq. (2.32) so that the sums over \mathbf{K} and \mathbf{L} are restricted to the region in which $K_z > L_z > 0$.

¹⁴ A. A. Broyles, Z. Physik 151, 187 (1958).

Finally, we make the transformation

$$\mathbf{X}(\mathbf{K}) = \mathbf{A}(\mathbf{K}) \mathbf{Y}(\mathbf{K}), \quad (3.4)$$

where the $\mathbf{A}(\mathbf{K})$ are $n \times n$ real symmetric matrices whose elements $a_{\alpha\beta}(\mathbf{K})$ satisfy the relation

$$a_{\alpha\gamma}(\mathbf{K}) a_{\gamma\beta}(\mathbf{K}) = \sigma_{\alpha\beta}(\mathbf{K}) = \int x_\alpha(\mathbf{K}) x_\beta(\mathbf{K}) \psi_0^2 d\tau, \quad (3.5)$$

and the $x_\alpha(\mathbf{K})$ are the elements of the column vector $\mathbf{X}(\mathbf{K})$. Using this transformation in Eq. (3.3) we obtain

$$I[G(\mathbf{Y})] = \int G(\mathbf{Y}) \exp \left\{ -\frac{1}{2} \sum_{\mathbf{K}} \mathbf{Y}^\dagger(\mathbf{K}) \times [\mathbf{A}(\mathbf{K}) \Phi(\mathbf{K}) \mathbf{A}(\mathbf{K})] \mathbf{Y}(\mathbf{K}) \right\} \psi_0^2 d\tau, \quad (3.6)$$

where

$$G(\mathbf{Y}) = F[\mathbf{P}\{\mathbf{A}(\mathbf{K}) \mathbf{Y}(\mathbf{K})\}]. \quad (3.7)$$

This transformation is introduced in order to make $\int y_\alpha(\mathbf{K}) y_\beta(\mathbf{K}) \psi_0^2 d\tau = \delta_{\alpha\beta}$. The entire procedure is often referred to as the Gram-Charlier expansion¹⁴ and is designed to make the second and third terms in the expansion zero.

By introducing the Jacobian of the transformation from \mathbf{r} space to \mathbf{Y} space, Eq. (3.6) becomes

$$I[G(\mathbf{Y})] = \int G(\mathbf{Y}) \exp \left\{ -\frac{1}{2} \sum_{\mathbf{K}} \mathbf{Y}^\dagger(\mathbf{K}) \times [\mathbf{A}(\mathbf{K}) \Phi(\mathbf{K}) \mathbf{A}(\mathbf{K})] \mathbf{Y}(\mathbf{K}) \right\} J(\mathbf{Y}) d\mathbf{Y}, \quad (3.8)$$

where

$$d\mathbf{Y} = \prod_{\mathbf{K}} \prod_{\alpha} dy_{\alpha}(\mathbf{K}) = \prod_{\mathbf{K}} d\mathbf{Y}(\mathbf{K}), \quad (3.9)$$

and the Jacobian $J(\mathbf{Y})$ contains the unperturbed wave function ψ_0 , so that

$$\int F(\mathbf{Y}) J(\mathbf{Y}) d\mathbf{Y} = \int F(\mathbf{Y}) \psi_0^2 d\tau. \quad (3.10)$$

The problem has thus been reduced to that of finding an expression for $J(\mathbf{Y})$.

By expanding $J(\mathbf{Y})$ in a Hermite series¹⁴ and then using the generating function for Hermite polynomials, the Jacobian may be written

$$J(\mathbf{Y}) = \lim_{\mathbf{T} \rightarrow 0, \mathbf{W} \rightarrow 0} (\exp \hat{O}) \langle \lambda(\mathbf{WY}) \rangle_0 \exp \left\{ -\frac{1}{2} \sum_{\mathbf{K}} [\mathbf{Y}^\dagger(\mathbf{K}) \mathbf{Y}(\mathbf{K}) + \mathbf{T}^\dagger(\mathbf{K}) \mathbf{T}(\mathbf{K}) - 2\mathbf{T}^\dagger(\mathbf{K}) \mathbf{Y}(\mathbf{K})] \right\} \prod_{\mathbf{K}} (2\pi)^{-n/2}, \quad (3.11)$$

where $\mathbf{T}(\mathbf{K})$ and $\mathbf{W}(\mathbf{K})$ are column vectors with elements $t_\alpha(\mathbf{K})$ and $w_\alpha(\mathbf{K})$,

$$\hat{O} = \sum_{\mathbf{K}} \frac{\partial}{\partial w_\alpha(\mathbf{K})} \frac{\partial}{\partial t_\alpha(\mathbf{K})}, \quad (3.12)$$

and

$$\langle \lambda(WY) \rangle_0$$

$$= \int \exp\left\{\frac{1}{2} \sum_{\mathbf{K}} [2W^\dagger(\mathbf{K})Y(\mathbf{K}) - W^\dagger(\mathbf{K})W(\mathbf{K})]\right\} J(Y) dY \quad \text{and}$$

$$= \int \exp\left\{\frac{1}{2} \sum_{\mathbf{K}} [2W^\dagger(\mathbf{K})Y(\mathbf{K}) - W^\dagger(\mathbf{K})W(\mathbf{K})]\right\} \psi_0^2 d\tau. \quad (3.13)$$

By using Eq. (3.11) the integral of Eq. (3.8) can now be written as

$$I[G(Y)] = (\exp \hat{O}) \langle \lambda(WY) \rangle_0 \exp\left\{-\frac{1}{2} \sum_{\mathbf{K}} T^\dagger(\mathbf{K})T(\mathbf{K})\right\} \\ \times \int G(Y) \exp\left\{-\frac{1}{2} \sum_{\mathbf{K}} [Y^\dagger(\mathbf{K})(A(\mathbf{K})\Phi(\mathbf{K})A(\mathbf{K}) + I) \right. \\ \left. \times Y(\mathbf{K}) - 2T^\dagger(\mathbf{K})Y(\mathbf{K})]\right\} \prod_{\mathbf{K}} \frac{dY(\mathbf{K})}{(2\pi)^{n/2}}, \quad (3.14)$$

where I is the $n \times n$ unit matrix. By completing the square in the exponential term which appears under the integral, this expression can be written

$$I[G(Y)] = (\exp \hat{O}) \left\{ \int G(Y) \exp\left\{\frac{1}{2} \sum_{\mathbf{K}} [Y(\mathbf{K}) - T'(\mathbf{K})]^\dagger \right. \right. \\ \left. \times B(\mathbf{K})[Y(\mathbf{K}) - T'(\mathbf{K})]\right\} \prod_{\mathbf{K}} \frac{dY(\mathbf{K})}{(2\pi)^{n/2}} \left. \right\} \\ \times \exp\left\{\frac{1}{2} \sum_{\mathbf{K}} T^\dagger(\mathbf{K})[B^{-1}(\mathbf{K}) - I]T(\mathbf{K})\right\} \\ \times \langle \lambda(WY) \rangle_0, \quad (3.15) \quad \text{and}$$

where we have defined

$$B(\mathbf{K}) = A(\mathbf{K})\Phi(\mathbf{K})A(\mathbf{K}) + I \quad (3.16)$$

$$T'(\mathbf{K}) = B^{-1}(\mathbf{K})T(\mathbf{K}). \quad (3.17)$$

It is understood in Eqs. (3.14) and (3.15) that after operating with $\exp \hat{O}$, the $t_\alpha(\mathbf{K})$ and $w_\alpha(\mathbf{K})$ are to be set equal to zero. Note that Eq. (3.15) is a shorthand notation for an infinite series, since, in general, the operator $\exp \hat{O}$ must be expanded as

$$\exp \hat{O} = \sum_{j=0}^{\infty} \frac{1}{j!} \hat{O}^j. \quad (3.18)$$

B. Energy Expansion

If we write Eq. (2.32) in terms of the real variables $y_\alpha(\mathbf{K})$, we obtain

$$E = E_0 - E_S + \frac{\hbar^2}{8m_1V} \sum_{\mathbf{K}} K^2 [\phi_{\alpha\beta}(\mathbf{K})g_{\beta}\phi_{\beta\gamma}(\mathbf{K}) + \mu_{\alpha\gamma}(\mathbf{K})] \\ \times F_{\alpha\gamma}(\mathbf{K}) + \frac{\hbar^2}{2m_1V^2} \sum_{\mathbf{K}, \mathbf{L} > \mathbf{L} > 0} \mathbf{K} \cdot \mathbf{L} \phi_{\alpha\beta}(\mathbf{K}) \frac{m_1}{m_\beta} \\ \times \phi_{\beta\gamma}(\mathbf{L}) G_{\alpha\beta\gamma}(\mathbf{KL}), \quad (3.19)$$

where

$$F_{\alpha\gamma}(\mathbf{K}) = V a_{\alpha\epsilon}(\mathbf{K}) \langle y_\epsilon(\mathbf{K}) y_\gamma(\mathbf{K}) \rangle a_{\gamma\gamma}(\mathbf{K}) \quad (3.20)$$

$$G_{\alpha\beta\gamma}(\mathbf{KL}) = \left(\frac{1}{2}V\right)^{3/2} \{ a_{\alpha\epsilon}(\mathbf{K}) [a_{\beta\gamma}(\mathbf{K} + \mathbf{L}) \langle y_\epsilon(\mathbf{K}) y_\gamma(\mathbf{K} + \mathbf{L}) y_\xi(\mathbf{L}) + y_\epsilon(\mathbf{K}) y_\gamma(-\mathbf{K} - \mathbf{L}) y_\xi(-\mathbf{L}) + y_\epsilon(-\mathbf{K}) y_\gamma(-\mathbf{K} - \mathbf{L}) y_\xi(\mathbf{L}) \\ - y_\epsilon(-\mathbf{K}) y_\gamma(\mathbf{K} + \mathbf{L}) y_\xi(-\mathbf{L})] - a_{\beta\gamma}(\mathbf{K} - \mathbf{L}) \langle y_\epsilon(\mathbf{K}) y_\gamma(\mathbf{K} - \mathbf{L}) y_\xi(\mathbf{L}) + y_\epsilon(-\mathbf{K}) y_\gamma(\mathbf{K} - \mathbf{L}) y_\xi(-\mathbf{L}) \\ + y_\epsilon(-\mathbf{K}) y_\gamma(-\mathbf{K} + \mathbf{L}) y_\xi(\mathbf{L}) - y_\epsilon(\mathbf{K}) y_\gamma(-\mathbf{K} + \mathbf{L}) y_\xi(-\mathbf{L}) \rangle] a_{\xi\gamma}(\mathbf{K}) \}. \quad (3.21)$$

Equation (3.15) can now be used to evaluate the averages in Eqs. (3.20) and (3.21). The evaluation of the resulting integrals is straightforward but somewhat tedious. These integrals are performed in Appendix A, with the result

$$F_{\alpha\gamma}(\mathbf{K}) = V a_{\alpha\epsilon}(\mathbf{K}) (\exp \hat{O}) [b_{\epsilon\delta}^{-1}(\mathbf{K}) + t_\epsilon'(\mathbf{K}) t_\delta'(\mathbf{K})] \exp\left\{\frac{1}{2} \sum_{\mathbf{N}} T^\dagger(\mathbf{N}) [B^{-1}(\mathbf{N}) - I] T(\mathbf{N})\right\} \langle \lambda(WY) \rangle_0 a_{\gamma\gamma}(\mathbf{K}) \\ \times ((\exp \hat{O}) \exp\left\{\frac{1}{2} \sum_{\mathbf{N}} T^\dagger(\mathbf{N}) [B^{-1}(\mathbf{N}) - I] T(\mathbf{N})\right\} \langle \lambda(WY) \rangle_0)^{-1} \quad (3.22)$$

and

$$G_{\alpha\beta\gamma}(\mathbf{KL}) = \left(\frac{1}{2}V\right)^{3/2} a_{\alpha\epsilon}(\mathbf{K}) (\exp \hat{O}) \{ a_{\beta\gamma}(\mathbf{K} + \mathbf{L}) [t_\epsilon'(\mathbf{K}) t_\gamma'(\mathbf{K} + \mathbf{L}) t_\xi'(\mathbf{L}) + t_\epsilon'(\mathbf{K}) t_\gamma'(-\mathbf{K} - \mathbf{L}) t_\xi'(-\mathbf{L}) \\ + t_\epsilon'(-\mathbf{K}) t_\gamma'(-\mathbf{K} - \mathbf{L}) t_\xi'(\mathbf{L}) - t_\epsilon'(-\mathbf{K}) t_\gamma'(\mathbf{K} + \mathbf{L}) t_\xi'(-\mathbf{L})] - a_{\beta\gamma}(\mathbf{K} - \mathbf{L}) [t_\epsilon'(\mathbf{K}) t_\gamma'(\mathbf{K} - \mathbf{L}) t_\xi'(\mathbf{L}) \\ + t_\epsilon'(-\mathbf{K}) t_\gamma'(\mathbf{K} - \mathbf{L}) t_\xi'(-\mathbf{L}) + t_\epsilon'(-\mathbf{K}) t_\gamma'(-\mathbf{K} + \mathbf{L}) t_\xi'(\mathbf{L}) - t_\epsilon'(\mathbf{K}) t_\gamma'(-\mathbf{K} + \mathbf{L}) t_\xi'(-\mathbf{L})] \} \\ \times (\exp\left\{\frac{1}{2} \sum_{\mathbf{N}} T^\dagger(\mathbf{N}) [B^{-1}(\mathbf{N}) - I] T(\mathbf{N})\right\} \langle \lambda(WY) \rangle_0) a_{\xi\gamma}(\mathbf{L}) \\ \times ((\exp \hat{O}) \exp\left\{\frac{1}{2} \sum_{\mathbf{N}} T^\dagger(\mathbf{N}) [B^{-1}(\mathbf{N}) - I] T(\mathbf{N})\right\} \langle \lambda(WY) \rangle_0)^{-1}. \quad (3.23)$$

The formal expression for the energy given by Eq. (3.19) in conjunction with Eqs. (3.21) and (3.22) is complicated, to say the least. Fortunately, much of this complexity disappears if one examines the energy expansion term by term. In Appendix B, the first several terms of this expansion are calculated. The energy expression obtained by retaining terms out to $j=3$ in the expansion of the operator $\exp\hat{O}$, Eq. (3.18), is sufficient to illustrate the nature of the expansion. Also, since in practice we are limited to systems for which H_0 and ψ_0 , Eq. (2.5), represent n ideal quantum gases, we shall restrict ourselves to that case. This restriction results in some simplification of the energy expression which, by retaining terms out to $j=3$ in the expansion of $\exp\hat{O}$, is

$$E = E_0 - E_S + \frac{\hbar^2}{8m_1} \sum_{\mathbf{K}} K^2 [\phi_{\alpha\beta}(\mathbf{K}) g_{\beta\gamma} \phi_{\beta\gamma}(\mathbf{K}) + \mu_{\alpha\gamma}(\mathbf{K})] \times d_{\alpha\gamma}^{-1}(\mathbf{K}) - \frac{\hbar^2}{8m_1 V^2} \sum'_{\mathbf{K}, \mathbf{L}} \mathbf{K} \cdot \mathbf{L} \phi_{\alpha\beta}(\mathbf{K}) \frac{m_1}{m_\beta} \phi_{\beta\gamma}(\mathbf{L}) d_{\alpha\epsilon}^{-1}(\mathbf{K}) \times d_{\beta\epsilon}^{-1}(\mathbf{K} + \mathbf{L}) d_{\gamma\epsilon}^{-1}(\mathbf{L}) \sigma_{\epsilon\epsilon}^{-1}(\mathbf{K}) \sigma_{\epsilon\epsilon}^{-1}(\mathbf{K} + \mathbf{L}) \sigma_{\epsilon\epsilon}^{-1}(\mathbf{L}) \times \langle \rho_\epsilon(\mathbf{K}) \rho_\epsilon^*(\mathbf{K} + \mathbf{L}) \rho_\epsilon(\mathbf{L}) \rangle_0, \quad (3.24)$$

where the $d_{\alpha\gamma}^{-1}(\mathbf{K})$ are the elements of the matrix $\mathbf{D}^{-1}(\mathbf{K})$ which is the inverse of the matrix $\mathbf{D}(\mathbf{K})$ whose elements are given by

$$d_{\alpha\gamma}(\mathbf{K}) = [\phi_{\alpha\gamma}(\mathbf{K}) + \sigma_{\alpha\gamma}^{-1}(\mathbf{K})]. \quad (3.25)$$

It is important to realize that the only unknown quantities which appear in Eq. (3.24) are the $\phi_{\alpha\beta}(\mathbf{K})$. A discussion of the $\sigma_{\alpha\gamma}(\mathbf{K})$ and the $\langle \rho_\epsilon(\mathbf{K}) \rho_\epsilon^*(\mathbf{K} + \mathbf{L}) \rho_\epsilon(\mathbf{L}) \rangle_0$ is given in Appendix C. While the complexity of the higher-order terms in the energy expansion increases rather rapidly, they too contain only the $\phi_{\alpha\beta}(\mathbf{K})$ as unknowns.

In Eq. (3.24), E_0 is the energy of a mixture of n ideal quantum gases and, as mentioned earlier, E_S is a self-energy term. The next term arises from the $j=0$ term in the expansion of $\exp\hat{O}$ and is the first approximation to the two-body interactions. The last term in Eq. (3.24) arises from $j=3$ in the expansion of $\exp\hat{O}$, and it is the first approximation to the three-body interactions. The terms which arise from $j=1$ and $j=2$ are zero.

It is now possible, in principle, to express the energy to any desired order in the expansion of $\exp\hat{O}$, minimize it with respect to variations in the $\phi_{\alpha\beta}(\mathbf{K})$, and thereby obtain the energy correct to any desired order in the expansion. This procedure is easy to carry out if one terminates the energy expansion after the first approximation to the two-body interactions.

Once the $\phi_{\alpha\beta}(\mathbf{K})$ have been determined, the wave function can be obtained from Eqs. (2.6) and (2.16), and is given by

$$\psi = \psi_0 \exp \left\{ -\frac{1}{2V} \sum_{\mathbf{K}} \sum_{i=1}^{N_\alpha} \sum_{j=1}^{N_\beta} e^{-i\mathbf{K} \cdot \mathbf{r}_{\alpha i}} \phi_{\alpha\beta}(\mathbf{K}) e^{i\mathbf{K} \cdot \mathbf{r}_{\beta j}} \right\}. \quad (3.26)$$

IV. VARIATION

The lowest-order approximation to the energy beyond the ideal quantum gas arises from the $j=0$ term in the expansion of $(\exp\hat{O})$ in Eq. (3.24), and is given by

$$E = E_0 - E_S + \frac{\hbar^2}{8m_1} \sum_{\mathbf{K}} K^2 [\phi_{\alpha\beta}(\mathbf{K}) g_{\beta\gamma} \phi_{\beta\gamma}(\mathbf{K}) + \mu_{\alpha\gamma}(\mathbf{K})] d_{\alpha\gamma}^{-1}(\mathbf{K}). \quad (4.1)$$

Since the $j=1$ and $j=2$ terms are zero, this expression is correct out through the $j=2$ term. This approximation is equivalent to approximating the Jacobian Eq. (3.11) by a Gaussian. Note that Eq. (4.1) is the same as the expression that is obtained by making *both* the RPA and the BS approximation.

If we use Eq. (3.25) to express Eq. (4.1) in terms of the $d_{\alpha\beta}(\mathbf{K})$ and the $d_{\alpha\beta}^{-1}(\mathbf{K})$, we get

$$E = E_0 - E_S + \frac{\hbar^2}{8m_1} \sum_{\mathbf{K}} K^2 \{ g_{\alpha\alpha} [d_{\alpha\alpha}(\mathbf{K}) - 2\sigma_{\alpha\alpha}^{-1}(\mathbf{K})] + d_{\alpha\beta}^{-1}(\mathbf{K}) c_{\beta\alpha}(\mathbf{K}) \}, \quad (4.2)$$

where

$$c_{\alpha\beta}(\mathbf{K}) = \sigma_{\alpha\gamma}^{-1}(\mathbf{K}) g_{\gamma\sigma} \sigma_{\gamma\beta}^{-1}(\mathbf{K}) + \mu_{\alpha\beta}(\mathbf{K}). \quad (4.3)$$

If we bear in mind that $\Phi(\mathbf{K})$ is a symmetric matrix, so that

$$\phi_{\alpha\beta}(\mathbf{K}) = \phi_{\beta\alpha}(\mathbf{K}), \quad (4.4)$$

it is easy to show that

$$\begin{aligned} \partial d_{\gamma\epsilon}(\mathbf{K}) / \partial \phi_{\alpha\beta}(\mathbf{K}) &= \delta_{\gamma\alpha} \delta_{\epsilon\beta} + \delta_{\gamma\beta} \delta_{\epsilon\alpha}, \quad \alpha \neq \beta \\ \partial d_{\gamma\epsilon}(\mathbf{K}) / \partial \phi_{\alpha\alpha}(\mathbf{K}) &= \delta_{\gamma\alpha} \delta_{\epsilon\alpha}, \end{aligned} \quad (4.5)$$

and

$$\begin{aligned} \partial d_{\gamma\epsilon}^{-1}(\mathbf{K}) / \partial \phi_{\alpha\beta}(\mathbf{K}) &= d_{\gamma\alpha}^{-1}(\mathbf{K}) d_{\epsilon\beta}^{-1}(\mathbf{K}) \\ &\quad + d_{\gamma\beta}^{-1}(\mathbf{K}) d_{\alpha\epsilon}^{-1}(\mathbf{K}), \quad \alpha \neq \beta \\ d_{\gamma\epsilon}^{-1}(\mathbf{K}) / \partial \phi_{\alpha\alpha}(\mathbf{K}) &= d_{\gamma\alpha}^{-1}(\mathbf{K}) d_{\alpha\epsilon}^{-1}(\mathbf{K}). \end{aligned} \quad (4.6)$$

If we now minimize Eq. (4.2) with respect to variations in the $\phi_{\alpha\beta}(\mathbf{K})$ by making use of Eqs. (4.5) and (4.6), we obtain

$$g_{\gamma} \delta_{\gamma\epsilon} - d_{\gamma\alpha}^{-1}(\mathbf{K}) c_{\alpha\beta}(\mathbf{K}) d_{\beta\epsilon}^{-1}(\mathbf{K}) = 0, \quad (4.7)$$

which can be written as

$$d_{\alpha\gamma}(\mathbf{K}) g_{\gamma} d_{\gamma\beta}(\mathbf{K}) - c_{\alpha\beta}(\mathbf{K}) = 0. \quad (4.8)$$

By using Eqs. (4.8) and (4.2), we can write the energy as

$$E = E_0 - E_S + \frac{\hbar^2}{4m_1} \sum_{\mathbf{K}} K^2 g_{\alpha} [d_{\alpha\alpha}(\mathbf{K}) - \sigma_{\alpha\alpha}^{-1}(\mathbf{K})]. \quad (4.9)$$

We must now solve Eq. (4.8). In general, this is by no means a trivial task. In Sec. V, we shall give the

solutions to Eq. (4.8) for a two-species system, and then use these solutions for the analysis of a system of electrons and nuclei at high densities.

V. TWO-SPECIES SYSTEM

In this section, we shall consider the solution to Eq. (4.8) for a two-species system. For the two-species system, Eq. (4.8) is given by

$$\begin{aligned} g_1 d_{11}^2(\mathbf{K}) + g_2 d_{12}^2(\mathbf{K}) &= c_{11}(\mathbf{K}), \\ \{g_1 d_{11}(\mathbf{K}) + g_2 d_{22}(\mathbf{K})\} d_{12}(\mathbf{K}) &= c_{12}(\mathbf{K}), \\ g_1 d_{12}^2(\mathbf{K}) + g_2 d_{22}^2(\mathbf{K}) &= c_{22}(\mathbf{K}). \end{aligned} \quad (5.1)$$

It is easy to show by direct substitution that Eq. (5.1) has the set of solutions given by

$$\begin{aligned} d_{11}(\mathbf{K}) &= \{c_{11}(\mathbf{K}) \\ &\quad + [(c_{11}(\mathbf{K})c_{22}(\mathbf{K}) - c_{12}^2(\mathbf{K}))g_2/g_1]^{1/2}\}/f(\mathbf{K}), \\ d_{12}(\mathbf{K}) &= c_{12}(\mathbf{K})/f(\mathbf{K}), \\ \text{and} \\ d_{22}(\mathbf{K}) &= \{c_{22}(\mathbf{K}) \\ &\quad + [(c_{11}(\mathbf{K})c_{22}(\mathbf{K}) - c_{12}^2(\mathbf{K}))g_1/g_2]^{1/2}\}/f(\mathbf{K}), \end{aligned} \quad (5.2)$$

where

$$f(\mathbf{K}) = \{g_1 c_{11}(\mathbf{K}) + 2[g_1 g_2 (c_{11}(\mathbf{K})c_{22}(\mathbf{K}) - c_{12}^2(\mathbf{K}))]^{1/2} + g_2 c_{22}(\mathbf{K})\}^{1/2}.$$

Using Eqs. (4.9) and (5.2), the expression for the energy becomes

$$E = E_0 - E_S + \frac{\hbar^2}{4m_1} \sum_{\mathbf{K}} K^2 [f(\mathbf{K}) - g_1 \sigma_{11}^{-1}(\mathbf{K}) - g_2 \sigma_{22}^{-1}(\mathbf{K})]. \quad (5.3)$$

We can now proceed in a straightforward manner to calculate the energy from Eq. (5.3) by using Eq. (4.3) for the $c_{\alpha\beta}(\mathbf{K})$. In general, the sum over \mathbf{K} (to be converted into an integral) must be done numerically.

For our application to a system of electrons and nuclei, it is perhaps more informative to rearrange Eq. (5.3) into a form which is more easily analyzed. To that end, we note that by adding and subtracting $2[g_1 g_2 c_{11}(\mathbf{K})c_{22}(\mathbf{K})]^{1/2}$, we can write

$$f(\mathbf{K}) = \{[g_1 c_{11}(\mathbf{K})]^{1/2} + [g_2 c_{22}(\mathbf{K})]^{1/2}\} \times \left\{ 1 - 2 \frac{[g_1 g_2 c_{11}(\mathbf{K})c_{22}(\mathbf{K})]^{1/2} - [g_1 g_2 (c_{11}(\mathbf{K})c_{22}(\mathbf{K}) - c_{12}^2(\mathbf{K}))]^{1/2}}{\{[g_1 c_{11}(\mathbf{K})]^{1/2} + [g_2 c_{22}(\mathbf{K})]^{1/2}\}^2} \right\}^{1/2}. \quad (5.4)$$

We can now expand Eq. (5.4) in a Taylor series to give

$$f(\mathbf{K}) = \left\{ [g_1 c_{11}(\mathbf{K})]^{1/2} + [g_2 c_{22}(\mathbf{K})]^{1/2} - \left[\frac{[g_1 g_2 c_{11}(\mathbf{K})c_{22}(\mathbf{K})]^{1/2} - [g_1 g_2 (c_{11}(\mathbf{K})c_{22}(\mathbf{K}) - c_{12}^2(\mathbf{K}))]^{1/2}}{[g_1 c_{11}(\mathbf{K})]^{1/2} + [g_2 c_{22}(\mathbf{K})]^{1/2}} \right] + \dots \right\}. \quad (5.5)$$

If we now choose $m_1 < m_2$ and note that in most cases m_1 will be much less than m_2 (for example, in a hydrogen plasma m_1 is the mass of an electron, while m_2 is the mass of a proton), then $g_2 \ll 1$, and a good approximation to $f(\mathbf{K})$ is given by the first two terms in Eq. (5.5). Using this approximation for $f(\mathbf{K})$, the energy becomes

$$\begin{aligned} E = & \left\{ E_{0m_1} + \frac{\hbar^2}{4m_1} \sum_{\mathbf{K}} K^2 [[g_1 c_{11}(\mathbf{K})]^{1/2} - g_1 \sigma_{11}^{-1}(\mathbf{K}) - \frac{1}{2} \rho_1^0 \mu_{11}(\mathbf{K})] \right\} \\ & + \left\{ E_{0m_2} + \frac{\hbar^2}{4m_1} \sum_{\mathbf{K}} K^2 [[g_2 c_{22}(\mathbf{K})]^{1/2} - g_2 \sigma_{22}^{-1}(\mathbf{K}) - \frac{1}{2} \rho_1^0 \mu_{22}(\mathbf{K})] \right\} \\ & - \frac{\hbar^2}{4m_1} \sum_{\mathbf{K}} K^2 \left[\frac{[g_1 g_2 c_{11}(\mathbf{K})c_{22}(\mathbf{K})]^{1/2} - [g_1 g_2 (c_{11}(\mathbf{K})c_{22}(\mathbf{K}) - c_{12}^2(\mathbf{K}))]^{1/2}}{[g_1 c_{11}(\mathbf{K})]^{1/2} + [g_2 c_{22}(\mathbf{K})]^{1/2}} \right]. \end{aligned} \quad (5.6)$$

Here we have used Eq. (2.28) to write

$$E_s = -\frac{\hbar^2}{4m_1} \sum_{\mathbf{K}} K^2 \left[\frac{1}{2} \rho_1^0 \mu_{11}(\mathbf{K}) + \frac{1}{2} \rho_2^0 \mu_{11}(\mathbf{K}) \right] \quad (5.7)$$

and

$$E_0 = E_{0m_1} + E_{0m_2}, \quad (5.8)$$

where E_{0m_1} is the energy of an ideal quantum gas of particles of mass m_1 and E_{0m_2} is the corresponding quantity for particles of mass m_2 .

The energy expression is now in an interesting form, which is easy to interpret. The terms enclosed by the first set of brackets depend only upon the particles of mass m_1 and the interaction between the particles of mass m_1 . For example, if the particles of mass m_1 are electrons, which interact through the Coulomb force, then the terms in the first set of brackets are simply the energy of a quantum electron gas. Likewise, the terms enclosed by the second set of brackets depend only upon the particles of mass m_2 and the interaction between the

particles of mass m_2 . The last term in Eq. (5.6) is a result of the interaction between the two species of particles. Note that if species (1) does not interact with species (2), that is, if $c_{12}(\mathbf{K})=0$, then this last term is zero.

We shall now consider Eq. (5.6) for a system which is composed of ZN electrons and N nuclei, where the charge on the nuclei is Ze , e being the magnitude of the charge of an electron. Species (1) is taken to be the electrons, while species (2) is composed of the nuclei. From Appendix C we have

$$\sigma_{\alpha\beta}(\mathbf{K}) = \rho_\alpha^0 S_\alpha(\mathbf{K}) \delta_{\alpha\beta}, \quad (5.9)$$

where $S_\alpha(\mathbf{K})$ is the structure factor for the ideal quantum gas composed of particles of mass m_α . Thus from

Eq. (4.3) we have

$$\begin{aligned} c_{11}(\mathbf{K}) &= [1/\rho_1^0 S_1^2(\mathbf{K})][1 + \rho_1^0 \mu_{11}(\mathbf{K}) S_1^2(\mathbf{K})], \\ c_{12}(\mathbf{K}) &= \mu_{12}(\mathbf{K}), \end{aligned} \quad (5.10)$$

and

$$c_{22}(\mathbf{K}) = [\delta/\rho_2^0 S_2^2(\mathbf{K})][1 + \rho_2^0 \mu_{22}(\mathbf{K}) S_2^2(\mathbf{K})/\delta],$$

where we have defined $\delta = m_1/m_2$. If we also use Eq. (2.29) to calculate

$$\mu_{11}(\mathbf{K}) = \frac{1}{Z^2} \mu_{22}(\mathbf{K}) = -\frac{1}{Z} \mu_{12}(\mathbf{K}) = \frac{16\pi m_1 e^2}{\hbar^2 K^4}, \quad (5.11)$$

then by using Eqs. (5.6), (5.10), and (5.11) the energy becomes

$$\begin{aligned} E = & \left(E_{0m_1} + \frac{\hbar^2}{4m_1} \sum_{\mathbf{K}} \frac{K^2}{S_1(\mathbf{K})} \{ [1 + \nu_{11}(\mathbf{K}) S_1^2(\mathbf{K})]^{1/2} - 1 - \frac{1}{2} \nu_{11}(\mathbf{K}) S_1(\mathbf{K}) \} \right) \\ & + \left(E_{0m_2} + \frac{\hbar^2}{4m_2} \sum_{\mathbf{K}} \frac{K^2}{S_2(\mathbf{K})} \{ [1 + \nu_{22}(\mathbf{K}) S_2^2(\mathbf{K})]^{1/2} - 1 - \frac{1}{2} \nu_{22}(\mathbf{K}) S_2(\mathbf{K}) \} \right) \\ & - \left(\frac{\hbar^2}{4m_1} \sum_{\mathbf{K}} \delta K^2 \{ [(1 + \nu_{11}(\mathbf{K}) S_1^2(\mathbf{K}))(1 + \nu_{22}(\mathbf{K}) S_2^2(\mathbf{K}))]^{1/2} - [1 + \nu_{11}(\mathbf{K}) S_1^2(\mathbf{K}) + \nu_{22}(\mathbf{K}) S_2^2(\mathbf{K})]^{1/2} \} \right. \\ & \left. \times \{ S_2(\mathbf{K}) [1 + \nu_{11}(\mathbf{K}) S_1^2(\mathbf{K})]^{1/2} + \delta S_1(\mathbf{K}) [1 + \nu_{22}(\mathbf{K}) S_2^2(\mathbf{K})]^{1/2} - 1 \} \right), \end{aligned} \quad (5.12)$$

where $\nu_{11}(\mathbf{K}) = \rho_1^0 \mu_{11}(\mathbf{K})$ and $\mu_{22}(\mathbf{K}) = \rho_2^0 \mu_{22}(\mathbf{K})/\delta$.

The sums over \mathbf{K} in this equation are to be converted into integrals via the replacement

$$\sum_{\mathbf{K}} \rightarrow \frac{V}{(2\pi)^3} \int d\mathbf{K}. \quad (5.13)$$

The resulting integrals are quite complicated and must, in general, be evaluated numerically. In the limit of very high densities, however, a rather good approximation to the energy can be obtained. The terms enclosed by the first set of brackets have been evaluated by Gaskell⁶ in the limit of high densities, with the result that the energy per electron is given by

$$E_e = \frac{2}{3}(\alpha/r_s)^2 + \frac{1}{2}(3/\pi)\alpha/r_s + \frac{1}{16}(3/\pi)^2 \ln r_s. \quad (5.14)$$

Here the energy is measured in rydbergs, $\alpha = (9\pi/4)^{1/3}$, and r_s is the so-called ion-sphere radius given by r_0/a_0 , where a_0 is the Bohr radius and $r_0 = (3/4\pi\rho_1^0)^{1/3}$. For spin- $\frac{1}{2}$ nuclei, the terms enclosed by the second set of brackets differ from those in the first only through the mass. From the terms in the second set of brackets, the energy per nucleus is given by

$$E_n = \frac{2}{3}\delta \left(\frac{\alpha}{r_s} \right)^2 + \frac{1}{2}Z^2 \left(\frac{3}{\pi} \right) \frac{\alpha}{r_s} + \frac{1}{16}Z^4 \left(\frac{3}{\pi} \right)^2 \ln r_s. \quad (5.15)$$

The contribution to the energy from the last term in Eq. (5.12) is actually associated with both the electrons and nuclei. However, because of the very much greater mass of the nuclei, it is appropriate to view this contribution as resulting from an alteration in the electron wave function. We therefore choose to measure this energy with respect to the number of electrons. We thus find that in the limit of very high densities the interaction energy per electron is given by

$$E_{\text{int}} = \frac{Z^{4/3}}{4(1 + \delta/Z^{1/3})} \left(\frac{3}{\pi} \right)^2 \ln r_s. \quad (5.16)$$

The energies given in Eqs. (5.14) and (5.15) have been thoroughly discussed elsewhere.¹⁻⁵ We shall therefore simply recall that the first term in either Eq. (5.14) or Eq. (5.15) is the ideal gas energy, the second is the exchange energy, while the final term is the dominant contribution to the correlation energy at high densities. Most authors also include a constant term in these energies. This constant term is also present in our theory; however, we have neglected it in the evaluation of the integrals.

The interaction energy per electron given by Eq. (5.16) is of the same form as the electron or the nucleus correlation energy. This is not unexpected. Since we know there will be no direct exchange energy between

distinguishable particles, we therefore expect the first contribution to the interaction energy to arise from the same type of changes in the wave function which gave rise to the $\ln r_s$ terms in Eqs. (5.14) and (5.15).

It is interesting to compare Eq. (5.16), for the case $Z=1$, with the electron correlation energy. If we set $Z=1$, then Eq. (5.16) becomes

$$E_{\text{int}} = [1/4(1+\delta)](3/\pi)^2 \ln r_s. \quad (5.17)$$

Note that this energy is greater than the electron correlation energy by the factor $4/(1+\delta)$. A factor $2/(1+\delta)$ can be accounted for by reduced-mass considerations. This can be made clear by noting that when $\delta=1$, this factor is unity. The remaining factor of 2 is accounted for by the fact that in the electron-nucleus interaction we associated all of that energy with the electron, while in the electron-electron interaction we associated half of the energy with each electron. The factors of Z which appear in Eq. (5.16) arise from the difference in density and the difference in charge between the two species of particles.

One further point should perhaps be made. As was pointed out by Gaskell,⁵ the correlation energy obtained here differs from that obtained from perturbation theory.¹⁻⁴ The discrepancy is essentially the factor $(3/\pi)^2$; however, its source is unknown.

VI. CONCLUSIONS

A series expansion for the ground-state energy of a many-species quantum system which is correct to within the pair approximation for the effective potential has been obtained. We then illustrate a procedure by which this energy expansion can be minimized with respect to variations in the effective potential to obtain the ground-state energy for the system. Although we illustrate this procedure by carrying it out retaining only the lowest-order term in the energy expansion, it is possible, at least in principle, to carry this out to any desired order in the energy expansion. The computational difficulty becomes considerable if one attempts to go beyond the lowest-order approximation. However, we believe that it is possible to obtain some correction to the lowest-order approximation, perhaps by iterating from the solutions to the lowest-order approximation.

The solutions to the variational equations for the lowest-order approximation to the energy have been obtained for a two-species system. When these solutions are used to analyze a system composed of electrons and nuclei, it is found that its energy can be written as the sum of the electron-gas energy plus the nuclei-gas energy plus a term which represents the interaction between the electrons and the nuclei. In the limit of high densities these solutions appear to be consistent. However, at low densities, since the lowest-order approximation to the energy is equivalent to the RPA plus

the BS approximation, we would expect these solutions to be a rather poor representation of the system.

The work presented here is applicable only to the ground state of the system. While the ground state is of interest in itself, it also provides a check point for theories which treat the system at nonzero temperatures. We are presently attempting to treat multi-species systems at nonzero temperatures by effective-potential methods. The results of this work, plus the fact that the electron gas has already been treated in this manner,¹⁶ are very encouraging.

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APPENDIX A

In order to use Eq. (3.15) for the evaluation of $F_{\alpha\gamma}(\mathbf{K})$ and $G_{\alpha\beta\gamma}(\mathbf{KL})$, we must evaluate the integral

$$I'[G(\mathbf{Y})] = \int G(\mathbf{Y}) \exp\left\{-\frac{1}{2} \sum_{\mathbf{N}} [\mathbf{Y}(\mathbf{N}) - \mathbf{T}'(\mathbf{N})]^t \mathbf{B}(\mathbf{N})\right. \\ \left. \times [\mathbf{Y}(\mathbf{N}) - \mathbf{T}'(\mathbf{N})]\right\} \prod_{\mathbf{N}} \frac{d\mathbf{Y}(\mathbf{N})}{(2\pi)^{n/2}}, \quad (\text{A1})$$

where $G(\mathbf{Y})$ is the function appropriate to either $F_{\alpha\gamma}(\mathbf{K})$ or $G_{\alpha\beta\gamma}(\mathbf{KL})$. For $F_{\alpha\gamma}(\mathbf{K})$ the integral is

$$I'[y_{\alpha}(\mathbf{K})y_{\gamma}(\mathbf{K})] = \int [z_{\alpha}(\mathbf{K}) + t_{\alpha}'(\mathbf{K})][z_{\gamma}(\mathbf{K}) + t_{\gamma}'(\mathbf{K})] \\ \times \exp\left\{-\frac{1}{2} \sum_{\mathbf{N}} \mathbf{Z}^t(\mathbf{N}) \mathbf{B}(\mathbf{N}) \mathbf{Z}(\mathbf{N})\right\} \\ \times \prod_{\mathbf{N}} \frac{d\mathbf{Z}(\mathbf{N})}{(2\pi)^{n/2}}, \quad (\text{A2})$$

where

$$\mathbf{Z}(\mathbf{N}) = \mathbf{Y}(\mathbf{N}) - \mathbf{T}'(\mathbf{N}) \quad (\text{A3})$$

and the $t_{\alpha}'(\mathbf{N})$ are the elements of the column vector $\mathbf{T}'(\mathbf{N})$. If we note that because of the quadratic form in the exponential in Eq. (A2), only even powers of $z_{\alpha}(\mathbf{K})$ will contribute to the integral, then we have

$$I'[y_{\alpha}(\mathbf{K})y_{\gamma}(\mathbf{K})] = \int [z_{\alpha}(\mathbf{K})z_{\gamma}(\mathbf{K}) + t_{\alpha}'(\mathbf{K})t_{\gamma}'(\mathbf{K})] \\ \times \exp\left\{-\frac{1}{2} \sum_{\mathbf{N}} \mathbf{Z}^t(\mathbf{N}) \mathbf{B}(\mathbf{N}) \mathbf{Z}(\mathbf{N})\right\} \prod_{\mathbf{N}} \frac{d\mathbf{Z}(\mathbf{N})}{(2\pi)^{n/2}}. \quad (\text{A4})$$

Integrating this equation by parts yields

$$I'[y_{\alpha}(\mathbf{K})y_{\gamma}(\mathbf{K})] = [b_{\alpha\gamma}^{-1}(\mathbf{K}) + t_{\alpha}'(\mathbf{K})t_{\gamma}'(\mathbf{K})] \\ \times \int \exp\left\{-\frac{1}{2} \sum_{\mathbf{N}} \mathbf{Z}^t(\mathbf{N}) \mathbf{B}(\mathbf{N}) \mathbf{Z}(\mathbf{N})\right\} \prod_{\mathbf{N}} \frac{d\mathbf{Z}(\mathbf{N})}{(2\pi)^{n/2}}. \quad (\text{A5})$$

¹⁶ T. Dunn and A. A. Broyles, Phys. Rev. 157, 156 (1967).

Now, by using Eqs. (3.15), (3.20), and (A5), we have

$$F_{\alpha\gamma}(\mathbf{K}) = V \left(a_{\alpha\epsilon}(\mathbf{K}) (\exp \hat{O}) \{ [b_{\epsilon\epsilon}^{-1}(\mathbf{K}) + t_{\epsilon}'(\mathbf{K}) t_{\epsilon}'(\mathbf{K})] \exp[\frac{1}{2} \sum_{\mathbf{N}} \mathbf{T}^{\dagger}(\mathbf{N}) [\mathbf{B}^{-1}(\mathbf{N}) - \mathbf{I}] \mathbf{T}(\mathbf{N})] \langle \lambda(\mathbf{WY}) \rangle_0 \} a_{\epsilon\gamma}(\mathbf{K}) \right) \\ \times \{ (\exp \hat{O}) \exp[\frac{1}{2} \sum_{\mathbf{N}} \mathbf{T}^{\dagger}(\mathbf{N}) [\mathbf{B}^{-1}(\mathbf{N}) - \mathbf{I}] \mathbf{T}(\mathbf{N})] \langle \lambda(\mathbf{WY}) \rangle_0 \}^{-1}. \quad (\text{A6})$$

The denominator in this expression is obtained by noting that $Q = I[1]$.

The function $G_{\alpha\beta\gamma}(\mathbf{KL})$ is a sum of terms of the form

$$I'[\gamma_{\epsilon}(\mathbf{K}) \gamma_{\epsilon}(\mathbf{M}) \gamma_{\epsilon}(\mathbf{L})] = \int [z_{\epsilon}(\mathbf{K}) + t_{\epsilon}'(\mathbf{K})] [z_{\epsilon}(\mathbf{M}) + t_{\epsilon}'(\mathbf{M})] [z_{\epsilon}(\mathbf{L}) + t_{\epsilon}'(\mathbf{L})] \\ \times \exp\{-\frac{1}{2} \sum_{\mathbf{N}} \mathbf{Z}^{\dagger}(\mathbf{N}) \mathbf{B}(\mathbf{N}) \mathbf{Z}(\mathbf{N})\} \prod_{\mathbf{N}} \frac{d\mathbf{Z}(\mathbf{N})}{(2\pi)^{n/2}}. \quad (\text{A7})$$

Since only even powers of $z_{\epsilon}(\mathbf{K})$ contribute to the integral, this expression can be written

$$I'[\gamma_{\epsilon}(\mathbf{K}) \gamma_{\epsilon}(\mathbf{M}) \gamma_{\epsilon}(\mathbf{L})] = \int [z_{\epsilon}(\mathbf{K}) z_{\epsilon}(\mathbf{K}) t_{\epsilon}'(\mathbf{L}) \delta_{\mathbf{KM}} + z_{\epsilon}(\mathbf{K}) z_{\epsilon}(\mathbf{K}) t_{\epsilon}'(\mathbf{M}) \delta_{\mathbf{KL}} + z_{\epsilon}(\mathbf{L}) z_{\epsilon}(\mathbf{L}) t_{\epsilon}'(\mathbf{K}) \delta_{\mathbf{LM}} + t_{\epsilon}'(\mathbf{K}) t_{\epsilon}'(\mathbf{M}) t_{\epsilon}'(\mathbf{L})] \\ \times \exp[-\frac{1}{2} \sum_{\mathbf{N}} \mathbf{Z}^{\dagger}(\mathbf{N}) \mathbf{B}(\mathbf{N}) \mathbf{Z}(\mathbf{N})] \prod_{\mathbf{N}} \frac{d\mathbf{Z}(\mathbf{N})}{(2\pi)^{n/2}}. \quad (\text{A8})$$

Integrating this expression by parts yields

$$I'[\gamma_{\epsilon}(\mathbf{K}) \gamma_{\epsilon}(\mathbf{M}) \gamma_{\epsilon}(\mathbf{L})] = [\delta_{\mathbf{KM}} b_{\epsilon\epsilon}^{-1}(\mathbf{K}) t_{\epsilon}'(\mathbf{L}) + \delta_{\mathbf{KL}} b_{\epsilon\epsilon}^{-1}(\mathbf{K}) t_{\epsilon}'(\mathbf{M}) + \delta_{\mathbf{LM}} b_{\epsilon\epsilon}^{-1}(\mathbf{L}) t_{\epsilon}'(\mathbf{K}) + t_{\epsilon}'(\mathbf{K}) t_{\epsilon}'(\mathbf{M}) t_{\epsilon}'(\mathbf{L})] \\ \times \int \exp[-\frac{1}{2} \sum_{\mathbf{N}} \mathbf{Z}^{\dagger}(\mathbf{N}) \mathbf{B}(\mathbf{N}) \mathbf{Z}(\mathbf{N})] \prod_{\mathbf{N}} \frac{d\mathbf{Z}(\mathbf{N})}{(2\pi)^{n/2}}. \quad (\text{A9})$$

Finally, by using Eqs. (3.15), (3.21), and (A9), we have

$$G_{\alpha\beta\gamma}(\mathbf{KL}) = (\frac{1}{2} V)^{3/2} (a_{\alpha\epsilon}(\mathbf{K}) (\exp \hat{O}) \{ a_{\beta\epsilon}(\mathbf{K} + \mathbf{L}) [t_{\epsilon}'(\mathbf{K}) t_{\epsilon}'(\mathbf{K} + \mathbf{L}) t_{\epsilon}'(\mathbf{L}) + t_{\epsilon}'(\mathbf{K}) t_{\epsilon}'(-\mathbf{K} - \mathbf{L}) t_{\epsilon}'(-\mathbf{L}) + t_{\epsilon}'(-\mathbf{K}) \\ \times t_{\epsilon}'(-\mathbf{K} - \mathbf{L}) t_{\epsilon}'(\mathbf{L}) - t_{\epsilon}'(-\mathbf{K}) t_{\epsilon}'(\mathbf{K} + \mathbf{L}) t_{\epsilon}'(-\mathbf{L})] - a_{\beta\epsilon}(\mathbf{K} - \mathbf{L}) [t_{\epsilon}'(\mathbf{K}) t_{\epsilon}'(\mathbf{K} - \mathbf{L}) t_{\epsilon}'(\mathbf{L}) + t_{\epsilon}'(-\mathbf{K}) \\ \times t_{\epsilon}'(\mathbf{K} - \mathbf{L}) t_{\epsilon}'(-\mathbf{L}) + t_{\epsilon}'(-\mathbf{K}) t_{\epsilon}'(-\mathbf{K} + \mathbf{L}) t_{\epsilon}'(\mathbf{L}) - t_{\epsilon}'(\mathbf{K}) t_{\epsilon}'(-\mathbf{K} + \mathbf{L}) t_{\epsilon}'(-\mathbf{L})] \} \\ \times [\exp\{\frac{1}{2} \sum_{\mathbf{K}} \mathbf{T}^{\dagger}(\mathbf{N}) [\mathbf{B}^{-1}(\mathbf{N}) - \mathbf{I}] \mathbf{T}(\mathbf{N})\} \langle \lambda(\mathbf{WY}) \rangle_0] a_{\epsilon\gamma}(\mathbf{L})) \\ \times [(\exp \hat{O}) \exp\{\frac{1}{2} \sum_{\mathbf{K}} \mathbf{T}^{\dagger}(\mathbf{N}) [\mathbf{B}^{-1}(\mathbf{N}) - \mathbf{I}] \mathbf{T}(\mathbf{N})\} \langle \lambda(\mathbf{WY}) \rangle_0]^{-1}. \quad (\text{A10})$$

APPENDIX B

We now evaluate $F_{\alpha\gamma}(\mathbf{K})$ and $G_{\alpha\beta\gamma}(\mathbf{KL})$ out to order $j=3$ in the expansion of the operator $(\exp \hat{O})$. For this purpose, it is convenient to write

$$F_{\alpha\gamma}(\mathbf{K}) = \sum_{j=0}^{\infty} F_{\alpha\gamma}^j(\mathbf{K}) \quad (\text{B1})$$

and

$$G_{\alpha\beta\gamma}(\mathbf{KL}) = \sum_{j=0}^{\infty} G_{\alpha\beta\gamma}^j(\mathbf{KL}), \quad (\text{B2})$$

where the $F_{\alpha\gamma}^j(\mathbf{K})$ and $G_{\alpha\beta\gamma}^j(\mathbf{KL})$ are the terms which arise from \hat{O}^j . We first note that $F_{\alpha\gamma}(\mathbf{K})$ contains only even powers of $t_{\alpha}'(\mathbf{K})$, and thus $F_{\alpha\gamma}^j(\mathbf{K})=0$ for all odd

values of j . Likewise, $G_{\alpha\beta\gamma}(\mathbf{KL})$ contains only odd powers of $t_{\alpha}'(\mathbf{K})$, and thus $G_{\alpha\beta\gamma}^j(\mathbf{KL})=0$ for all even values of j .

The $j=0$ terms are quite easily calculated. Since zero is even, $G_{\alpha\beta\gamma}^0(\mathbf{KL})$ is zero, and therefore

$$F_{\alpha\gamma}^0(\mathbf{K}) = V a_{\alpha\epsilon}(\mathbf{K}) b_{\epsilon\epsilon}^{-1}(\mathbf{K}) a_{\epsilon\gamma}(\mathbf{K}) = V d_{\alpha\gamma}^{-1}(\mathbf{K}), \quad (\text{B3})$$

where we have defined

$$d_{\alpha\gamma}^{-1}(\mathbf{K}) = a_{\alpha\epsilon}(\mathbf{K}) b_{\epsilon\epsilon}^{-1}(\mathbf{K}) a_{\epsilon\gamma}(\mathbf{K}). \quad (\text{B4})$$

As mentioned previously, the transformation via the matrix $\mathbf{A}(\mathbf{K})$ was designed to make the $j=1$ and $j=2$ terms zero.¹⁴ We are thus left with the calculation of $G_{\alpha\beta\gamma}^3(\mathbf{KL})$.

From Eq. (3.21) it is easy to see that $G_{\alpha\beta\gamma}^3(\mathbf{KL})$ is a

sum of terms of the form

$$R_{\alpha\beta\gamma}(\mathbf{KML}) = (\frac{1}{2}V)^{3/2} a_{\alpha\epsilon}(\mathbf{K}) a_{\beta\zeta}(\mathbf{M}) a_{\gamma\xi}(\mathbf{L}) (\hat{O}^3/3!) \\ \times [t_{\epsilon'}(\mathbf{K}) t_{\zeta'}(\mathbf{M}) t_{\xi'}(\mathbf{L}) \exp\{\frac{1}{2} \sum_{\mathbf{N}} \mathbf{T}^{\dagger}(\mathbf{N}) \\ \times [\mathbf{B}^{-1}(\mathbf{N}) - \mathbf{I}] \mathbf{T}(\mathbf{N})\} \langle \lambda(\mathbf{WY}) \rangle_0], \quad (\text{B5})$$

where we recall that

$$\hat{O}^3 = \lim_{\mathbf{W} \rightarrow 0, \mathbf{T} \rightarrow 0} \sum_{\mathbf{K}_1 \mathbf{K}_2 \mathbf{K}_3} \frac{\partial^3}{\partial t_{\alpha_1}(\mathbf{K}_1) \partial t_{\alpha_2}(\mathbf{K}_2) \partial t_{\alpha_3}(\mathbf{K}_3)} \\ \times \frac{\partial^3}{\partial w_{\alpha_1}(\mathbf{K}_1) \partial w_{\alpha_2}(\mathbf{K}_2) \partial w_{\alpha_3}(\mathbf{K}_3)}. \quad (\text{B6})$$

Straightforward application of the operator \hat{O}^3 yields

$$R_{\alpha\beta\gamma}(\mathbf{KML}) = (\frac{1}{2}V)^{3/2} a_{\alpha\epsilon}(\mathbf{K}) a_{\beta\zeta}(\mathbf{M}) a_{\gamma\xi}(\mathbf{L}) b_{\epsilon\alpha_1}^{-1}(\mathbf{K}) \\ \times b_{\zeta\alpha_2}^{-1}(\mathbf{M}) b_{\xi\alpha_3}^{-1}(\mathbf{L}) \langle y_{\alpha_1}(\mathbf{K}) y_{\alpha_2}(\mathbf{M}) y_{\alpha_3}(\mathbf{L}) \rangle_0, \quad (\text{B7})$$

where we have used the fact that

$$\langle y_{\alpha}(\mathbf{K}) \rangle_0 = 0. \quad (\text{B8})$$

Now by using the relations

$$y_{\alpha}(\mathbf{K}) = a_{\alpha\beta}^{-1}(\mathbf{K}) x_{\beta}(\mathbf{K}) \quad (\text{B9})$$

and

$$a_{\alpha\beta}(\mathbf{K}) a_{\beta\gamma}^{-1}(\mathbf{K}) = \delta_{\alpha\gamma}, \quad (\text{B10})$$

we can write Eq. (B7) as

$$R_{\alpha\beta\gamma}(\mathbf{KML}) = (\frac{1}{2}V)^{3/2} d_{\alpha\epsilon}^{-1}(\mathbf{K}) d_{\beta\zeta}^{-1}(\mathbf{M}) d_{\gamma\xi}^{-1}(\mathbf{L}) \\ \times \sigma_{\epsilon\alpha_1}^{-1}(\mathbf{K}) \sigma_{\zeta\alpha_2}^{-1}(\mathbf{M}) \sigma_{\xi\alpha_3}^{-1}(\mathbf{L}) \\ \times \langle x_{\alpha_1}(\mathbf{K}) x_{\alpha_2}(\mathbf{M}) x_{\alpha_3}(\mathbf{L}) \rangle_0. \quad (\text{B11})$$

Finally, by using the relationship between $x_{\alpha}(\mathbf{K})$ and $\rho_{\alpha}(\mathbf{K})$, substitution of Eq. (B11) with the appropriate values of \mathbf{K} , \mathbf{M} , and \mathbf{L} into Eq. (3.21) yields

$$G_{\alpha\beta\gamma}^3(\mathbf{KML}) = d_{\alpha\epsilon}^{-1}(\mathbf{K}) \sigma_{\epsilon\alpha_1}^{-1}(\mathbf{K}) \\ \times \{ d_{\beta\zeta}^{-1}(\mathbf{K}+\mathbf{L}) \sigma_{\zeta\alpha_2}^{-1}(\mathbf{K}+\mathbf{L}) \times \text{Re} \langle \rho_{\alpha_1}(\mathbf{K}) \rho_{\alpha_2}^*(\mathbf{K}+\mathbf{L}) \\ \times \rho_{\alpha_3}(\mathbf{L}) \rangle_0 - d_{\beta\zeta}^{-1}(\mathbf{K}-\mathbf{L}) \sigma_{\zeta\alpha_2}^{-1}(\mathbf{K}-\mathbf{L}) \\ \times \text{Re} \langle \rho_{\alpha_1}^*(\mathbf{K}) \rho_{\alpha_2}(\mathbf{K}-\mathbf{L}) \rho_{\alpha_3}(\mathbf{L}) \rangle_0 \} \\ \times \sigma_{\xi\alpha_3}^{-1}(\mathbf{D}) d_{\xi\gamma}^{-1}(\mathbf{L}). \quad (\text{B12})$$

If Eq. (B12) is used in Eq. (3.19) and the sum over the region in which $K_z > L_z > 0$ is extended to all values of \mathbf{K} and \mathbf{L} , then the last term in Eq. (3.19), which we will denote by E' , is given by

$$E' = -\frac{\hbar^2}{8m_1 V^2} \sum'_{\mathbf{KL}} \mathbf{K} \cdot \mathbf{L} \phi_{\alpha\beta}(\mathbf{K}) \frac{m_1}{m_{\beta}} \phi_{\beta\gamma}(\mathbf{L}) d_{\alpha\epsilon}^{-1}(\mathbf{K}) \\ \times d_{\beta\zeta}^{-1}(\mathbf{K}+\mathbf{L}) d_{\gamma\xi}^{-1}(\mathbf{L}) \sigma_{\epsilon\alpha_1}^{-1}(\mathbf{K}) \sigma_{\zeta\alpha_2}^{-1}(\mathbf{K}+\mathbf{L}) \sigma_{\xi\alpha_3}^{-1}(\mathbf{L}) \\ \times \langle \rho_{\alpha_1}(\mathbf{K}) \rho_{\alpha_2}^*(\mathbf{K}+\mathbf{L}) \rho_{\alpha_3}(\mathbf{L}) \rangle_0. \quad (\text{B13})$$

If ψ_0 represents a mixture of ideal quantum gases, then the $\sigma_{\alpha\beta}^{-1}(\mathbf{K})$ are the elements of a diagonal matrix and

$\langle \rho_{\alpha_1}(\mathbf{K}) \rho_{\alpha_2}^*(\mathbf{K}+\mathbf{L}) \rho_{\alpha_3}(\mathbf{L}) \rangle_0$ is zero unless $\alpha_1 = \alpha_2 = \alpha_3$. Thus, for this case,

$$E' = -\frac{\hbar^2}{8m_1 V^2} \sum'_{\mathbf{KL}} \mathbf{K} \cdot \mathbf{L} \phi_{\alpha\beta}(\mathbf{K}) \frac{m_1}{m_{\beta}} \phi_{\beta\gamma}(\mathbf{L}) d_{\alpha\epsilon}^{-1}(\mathbf{K}) \\ \times d_{\beta\epsilon}^{-1}(\mathbf{K}+\mathbf{L}) d_{\gamma\epsilon}^{-1}(\mathbf{L}) \sigma_{\epsilon\epsilon}^{-1}(\mathbf{K}) \sigma_{\epsilon\epsilon}^{-1}(\mathbf{K}+\mathbf{L}) \sigma_{\epsilon\epsilon}^{-1}(\mathbf{L}) \\ \times \langle \rho_{\epsilon}(\mathbf{K}) \rho_{\epsilon}^*(\mathbf{K}+\mathbf{L}) \rho_{\epsilon}(\mathbf{L}) \rangle_0. \quad (\text{B14})$$

APPENDIX C

We now present a brief discussion of the functions $\sigma_{\alpha\beta}(\mathbf{K})$ and $\langle \rho_{\alpha}(\mathbf{K}) \rho_{\beta}(\mathbf{K}+\mathbf{L}) \rho_{\gamma}(\mathbf{L}) \rangle_0$ for the case in which ψ_0 is the ground-state wave function for a mixture of ideal quantum gases. Using Eqs. (3.2) and (3.5), we can write

$$\sigma_{\alpha\beta}(\mathbf{K}) = \int x_{\alpha}(\mathbf{K}) x_{\beta}(\mathbf{K}) \psi_0^2 d\tau = \frac{1}{2V} \int [\rho_{\alpha}(\mathbf{K}) + \rho_{\alpha}^*(\mathbf{K})] \\ \times [\rho_{\beta}(\mathbf{K}) + \rho_{\beta}^*(\mathbf{K})] \psi_0^2 d\tau, \quad (\text{C1})$$

where $K_z > 0$. Since for a mixture of ideal gases different species do not interact with each other, $\sigma_{\alpha\beta}(\mathbf{K})$ is zero unless $\alpha = \beta$. Thus we have

$$\sigma_{\alpha\beta}(\mathbf{K}) = \delta_{\alpha\beta} \left\{ \frac{1}{V} \int \rho_{\alpha}(\mathbf{K}) \rho_{\alpha}^*(\mathbf{K}) \psi_0^2 d\tau \right. \\ \left. + \frac{1}{2V} \int [\rho_{\alpha}(\mathbf{K}) \rho_{\alpha}(\mathbf{K}) + \rho_{\alpha}^*(\mathbf{K}) \rho_{\alpha}^*(\mathbf{K})] \psi_0^2 d\tau \right\}. \quad (\text{C2})$$

It is easy to show that the last term in this expression is zero. (In this Appendix, we shall not employ the summation convention.)

By using Eq. (2.18), Eq. (C2) can be further simplified to

$$\sigma_{\alpha\beta}(\mathbf{K}) = \delta_{\alpha\beta} \frac{1}{V} \sum_{j=1}^{N_{\alpha}} \sum_{k=1}^{N_{\alpha}} e^{i\mathbf{K} \cdot (\mathbf{r}_{\alpha j} - \mathbf{r}_{\alpha k})} \psi_0^2 d\tau. \quad (\text{C3})$$

Using the definition of the pair-correlation function, this may be written

$$\sigma_{\alpha\beta}(\mathbf{K}) = \delta_{\alpha\beta} \left\{ \rho_{\alpha}^0 + \frac{1}{V^2} \sum_{j=1}^{N_{\alpha}} \sum_{k=1}^{N_{\alpha}} \int e^{i\mathbf{K} \cdot (\mathbf{r}_{\alpha j} - \mathbf{r}_{\alpha k})} g_{\alpha\alpha}^{(2)}(|\mathbf{r}_{\alpha j} - \mathbf{r}_{\alpha k}|) d\mathbf{r}_{\alpha j} d\mathbf{r}_{\alpha k} \right\}, \quad (\text{C4})$$

where, since we have assumed ψ_0^2 to be normalized,

$$g_{\alpha\alpha}^{(2)}(|\mathbf{r}_{\alpha j} - \mathbf{r}_{\alpha k}|) = V^2 \int \psi_0^2 d\tau' \quad (\text{C5})$$

is the pair-correlation function for the α th species, and the notation $d\tau'$ means that integration over $\mathbf{r}_{\alpha j}$ and $\mathbf{r}_{\alpha k}$ is omitted. Integration of Eq. (C4) yields

$$\sigma_{\alpha\beta}(\mathbf{K}) = \delta_{\alpha\beta} \rho_{\alpha}^0 [1 + \rho_{\alpha}^0 g_{\alpha\alpha}^{(2)}(\mathbf{K})] = \delta_{\alpha\beta} \rho_{\alpha}^0 S_{\alpha}(\mathbf{K}). \quad (\text{C6})$$

where $g_{\alpha\alpha}^{(2)}(\mathbf{K})$ is the Fourier transform of $g_{\alpha\alpha}^{(2)}(\mathbf{r})$ and $S_{\alpha}(\mathbf{K})$ is the structure factor for the α th species.

The structure factor for the ideal quantum gas has been evaluated elsewhere.¹⁶ If the α th species consists of spin- $\frac{1}{2}$ fermions with equal numbers of particles in the spin-up and spin-down states, then

$$S_{\alpha}(\mathbf{K}) = \frac{3}{4} x_{\alpha} (1 - \frac{1}{12} x_{\alpha}^2), \quad 0 \leq x_{\alpha} \leq 2$$

and

$$S_{\alpha}(\mathbf{K}) = 1, \quad 2 \leq x_{\alpha} \quad (\text{C7})$$

where

$$x_{\alpha} = K / (3\pi^2 \rho_{\alpha}^0)^{1/3}. \quad (\text{C8})$$

If the α th species consists of bosons, then

$$S_{\alpha}(\mathbf{K}) = 1 \quad (\text{C9})$$

for all values of \mathbf{K} .

Since the different species of a mixture of ideal gases do not interact, $\langle \rho_{\alpha}(\mathbf{K}) \rho_{\beta}^*(\mathbf{K} + \mathbf{L}) \rho_{\gamma}(\mathbf{L}) \rangle_0$ is zero unless $\alpha = \beta = \gamma$. We therefore direct our attention to the evaluation of

$$\begin{aligned} & \langle \rho_{\alpha}(\mathbf{K}) \rho_{\alpha}^*(\mathbf{K} + \mathbf{L}) \rho_{\alpha}(\mathbf{L}) \rangle_0 \\ &= \sum_{jkl}^{N_{\alpha}} \exp\{i[\mathbf{K} \cdot \mathbf{r}_{\alpha j} - (\mathbf{K} + \mathbf{L}) \cdot \mathbf{r}_{\alpha k} + \mathbf{L} \cdot \mathbf{r}_{\alpha l}]\} \psi_0^2 d\tau. \end{aligned} \quad (\text{C10})$$

¹⁶ See, e.g., T. Gaskell, Ref. 5.

This expression can be written as

$$\begin{aligned} & \langle \rho_{\alpha}(\mathbf{K}) \rho_{\alpha}^*(\mathbf{K} + \mathbf{L}) \rho_{\alpha}(\mathbf{L}) \rangle_0 \\ &= N_{\alpha} \{ 1 + \rho_{\alpha}^0 [g_{\alpha\alpha}^{(2)}(\mathbf{K}) + g_{\alpha\alpha}^{(2)}(\mathbf{K} + \mathbf{L}) + g_{\alpha\alpha}^{(2)}(\mathbf{L})] \} \\ & \quad + (\rho_{\alpha}^0)^3 \int \exp\{i[\mathbf{K} \cdot \mathbf{r}_1 - (\mathbf{K} + \mathbf{L}) \cdot \mathbf{r}_2 + \mathbf{L} \cdot \mathbf{r}_3]\} \\ & \quad \times g_{\alpha}^{(3)}(\mathbf{r}_1 \mathbf{r}_2 \mathbf{r}_3) d\mathbf{r}_1 d\mathbf{r}_2 d\mathbf{r}_3, \end{aligned} \quad (\text{C11})$$

where $g_{\alpha}^{(3)}(\mathbf{r}_1 \mathbf{r}_2 \mathbf{r}_3)$ is the three-body correlation function for the α th species.

For the ideal quantum gas, $g_{\alpha}^{(3)}(\mathbf{r}_1 \mathbf{r}_2 \mathbf{r}_3)$ is a known function. In fact, Lado¹⁷ has shown that the η -body correlation function $g_{\alpha}^{(\eta)}(\mathbf{r}_1 \mathbf{r}_2 \cdots \mathbf{r}_{\eta})$ for a system in which all the spin projections are parallel is given by

$$g_{\alpha}^{(\eta)}(\mathbf{r}_1 \mathbf{r}_2 \cdots \mathbf{r}_{\eta}) = \sum_P (\pm 1)^P \prod_{j=1}^{\eta} D_{\alpha}(\mathbf{r}_j - \mathbf{r}_{Pj}), \quad (\text{C12})$$

where \sum_P is a sum over all permutations of the η values of j , $(+1)^P$ is for bosons, and $(-1)^P$ is for fermions. The function $D_{\alpha}(\mathbf{r}_j - \mathbf{r}_k)$ is

$$D_{\alpha}(\mathbf{r}_j - \mathbf{r}_k) = \frac{1}{N_{\alpha}} \sum_{\mathbf{K}} n_{\alpha}(\mathbf{K}) e^{i\mathbf{K} \cdot (\mathbf{r}_j - \mathbf{r}_k)}, \quad (\text{C13})$$

where $n_{\alpha}(\mathbf{K})$ is the occupation number for particles with momentum $\hbar\mathbf{K}$ in the ground state of an ideal quantum gas of density ρ_{α}^0 . Since Eq. (C12) is for the case in which all of the particles have the same spin projection, if more than one spin projection is present in the α th species, then it must be averaged over all spin projections present.¹⁷

If higher-order terms are retained in the energy expansion, then Eq. (C12) can be used to evaluate explicitly the averages over ψ_0^2 which will appear in these higher-order terms.

¹⁷ F. Lado, J. Chem. Phys. 47, 5369 (1967); see, also, J. K. Jaen, J. Math. Phys. 8, 1483 (1967).